

# Localized magnetic states in metals

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Under certain conditions, the wave functions which are eigenfunctions of the Anderson Hamiltonian corresponding to magnetic and nonmagnetic states of the impurity atom are related to each other in a simple way. The differences between the energies of these states are determined by the poles of the two-particle electron-hole Green's function.

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1. In this letter we will show that under certain conditions there is a simple relationship between the wave functions of the magnetic and nonmagnetic states of an impurity which are determined by the Anderson Hamiltonian.<sup>1</sup> The necessary conditions reduce to the requirement that the distances between the energy levels of these states must be much larger than the energy of the interaction of the impurity with conduction electrons. In general, the wave functions of the magnetic and nonmagnetic states can be written in the form

$$\Phi = A_1 (a_{\sigma}^+ \psi_1 + a_{-\sigma}^+ \psi_1') + A_2 a_{\sigma}^+ i a_{-\sigma}^+ \psi_2 + A_3 \psi_3, \quad (1)$$

where the normalized function  $\phi_1$ ,  $\psi_1'$ ,  $\psi_2$ , and  $\psi_3$  describe the state of a degenerate

electron gas which is interacting with the impurity atom;  $a_{\sigma}^{+}$  is the operator which creates an electron at a localized  $d$  level with a spin  $\sigma$ ; and  $A_1, A_2$ , and  $A_3$  are constant coefficients. We will show below that the wave functions for the magnetic and non-magnetic states written in form (1) differ from each other only in the values of the coefficients  $A_1, A_2$ , and  $A_3$ . This is an exact conclusion and does not require ignoring any small quantities. Expression (1) gives the wave function  $\Phi$  of the entire system as a superposition of states in which the occupation numbers of the localized  $d$  level of the impurity atom are 1, 2, and 0. By "magnetic state" we mean one for which  $|A_1^{\text{mag}}|^2 > |A^{\text{nonmag}}|^2$ . The terms in (1) which are multiplied by the coefficient  $A_1$  correspond to those parts of  $\Phi$  which describe two opposite directions of the magnetic moment of the impurity atom. The spontaneous magnetic moment of the impurity in this "magnetic" state is zero.<sup>3,4</sup> The general properties of the wave functions of the magnetic and nonmagnetic states make it possible to relate the differences between the energies of these states with the poles of a two-particle electron-hole Green's function.

2. Using the commutation relations for  $a_{d\sigma}^{+}$  and  $a_{d\sigma}$ , which are the creation and annihilation operators for an electron in the impurity  $d$  level with spin  $\sigma$ , we rewrite the Anderson Hamiltonian<sup>1</sup> in the form

$$H = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} a_{\mathbf{k}\sigma}^{+} a_{\mathbf{k}\sigma} + \sum_{\sigma} \left( \epsilon_d + \frac{U}{2} \right) a_{d\sigma}^{+} a_{d\sigma} - \frac{U}{2} ( a_{d\sigma} a_{d\sigma}^{+} a_{d-\sigma}^{+} a_{d-\sigma} + a_{d\sigma}^{+} a_{d\sigma} a_{d-\sigma} a_{d-\sigma}^{+} ) + V \sum_{\mathbf{k}, \sigma} ( a_{\mathbf{k}\sigma}^{+} a_{d\sigma} + a_{d\sigma}^{+} a_{\mathbf{k}\sigma} ). \quad (2)$$

All the notations here are standard. When the Hamiltonian is written this way, the intra-atomic  $d$ - $d$  interaction appears in  $H$  only in the electron-hole interaction.

Let us assume that the constant of the  $s$ - $d$  interaction,  $V$ , is zero. We denote the rest of the Hamiltonian in (2) as  $H^0$ . The Schrödinger equation for  $H^0$  has solutions which are the wave functions for a system consisting of two noninteracting parts. One part corresponds to an isolated impurity atom, and the other to the degenerate electron gas.

We can construct three wave functions which describe the various magnetic states of the impurity atom under the condition that the degenerate electron gas is in the ground state. These functions and the corresponding energies are

$$\begin{aligned} \Phi_1^{\circ} &= \frac{1}{\sqrt{2}} ( a_{\sigma}^{+} + a_{-\sigma}^{+} ) |2N\rangle, & E_1^{\circ} &= 2E^{\circ} + \epsilon_d; \\ \Phi_2^{\circ} &= a_{\sigma}^{+} a_{-\sigma}^{+} |2N-1\rangle, & E_2^{\circ} &= 2E^{\circ} - \epsilon_F + 2\left( \epsilon_d + \frac{U}{2} \right); \\ \Phi_3^{\circ} &= |2N+1\rangle, & E_3^{\circ} &= 2E^{\circ} + \epsilon_F, \end{aligned} \quad (3)$$

where  $|2N\rangle$  is the ground state of a degenerate electron gas which contains  $N$  electrons with spin  $\sigma$  and  $N$  with spin  $-\sigma$ . In the state  $|2N-1\rangle$  there are  $2N-1$  particles. The one hole which forms in this state is distributed equiprobably over the Fermi surfaces corresponding to the spins  $\sigma$  and  $-\sigma$ . The notation  $|2N+1\rangle$  has a corresponding meaning. The quantity  $2E^{\circ}$  is the energy of the  $|2N\rangle$  ground state of the degenerate electron gas. The function  $\Phi_1^{\circ}$  describes a superposition of magnetic states of the

function  $\Phi_1^0$  describes a superposition of magnetic states of the impurity atom;  $\Phi_2^0$  corresponds to a nonmagnetic spin-singlet state; and  $\Phi_3^0$  corresponds to a nonmagnetic state of the impurity atom in which both of the  $d$  levels are vacant.

The  $s$ - $d$  interaction cannot be incorporated in Hamiltonian (2) by the methods of ordinary perturbation theory, even for values of  $V$  which physically are arbitrarily small. The reason is that  $V$  excites in a degenerate electron gas a large number of electron-hole pairs whose energies tend toward zero. When the interaction is turned on, the functions  $\Phi_1^0$ ,  $\Phi_2^0$ , and  $\Phi_3^0$  are mixed, and electron-hole pairs are excited.

3. Let us consider a nonmagnetic state of an impurity atom. The general expression for the wave function of the entire system for this state is of the form in (1). Substituting this expression into the Schrödinger equation, multiplying the result from the left by  $(a_\sigma^+ \psi_1)^+$ ,  $(a_\sigma^+ a_{-\sigma}^+ \psi_2)^+$ , and  $\psi_3^+$ , and integrating over the coordinates of all the particles, we find the following system of algebraic equations:

$$\begin{aligned} A_1 H_{11}^0 + A_2 V_{12} + A_3 V_{13} &= A_1 E, \\ A_2 H_{22}^0 + A_1 V_{21} + A_1 V_{21}' &= A_2 E, \\ A_3 H_{33}^0 + A_1 V_{31} + A_1 V_{31}' &= A_3 E, \end{aligned} \quad (4)$$

where  $H_{ii}^0$  is a diagonal matrix element of the operator  $H^0$ , and  $V_{ij}$  is a matrix element of the operator of the  $s$ - $d$  interaction, described by the last term in Hamiltonian (2). The matrix elements in (4) calculated with the wave functions  $a_\sigma^+ \Phi_1$  and  $a_{-\sigma}^+ \Phi_1'$  are respectively equal; i.e.,  $H_{11}^0 = H_{11'}^0$  and  $V_{i1} = V_{i1}'$ . System (4) thus contains only three equations. The secular equation for determining the eigenvalues of system (4) is

$$\begin{aligned} E^3 - E^2 (H_{11}^0 + H_{22}^0 + H_{33}^0) + E (H_{11}^0 H_{22}^0 + H_{11}^0 H_{33}^0 + H_{22}^0 H_{33}^0 - 2 |V_{12}|^2 \\ - 2 |V_{13}|^2) - H_{11}^0 H_{22}^0 H_{33}^0 + 2 |V_{12}|^2 H_{33}^0 + 2 |V_{13}|^2 H_{22}^0 = 0. \end{aligned} \quad (5)$$

If  $V = 0$ , the roots of this cubic equation are the quantities  $E_1^0$ ,  $E_2^0$ , and  $E_3^0$  given by (3).

According to the Cardan rule, a third-degree algebraic equation has three different real roots only if  $Q < 0$ , where

$$Q = \left(\frac{p}{3}\right)^3 + \left(\frac{q}{2}\right)^2; \quad p = -\frac{a^2}{3} + b \quad \text{and} \quad q = 2\left(\frac{a}{3}\right)^3 - \frac{ab}{3} + c.$$

The constants  $a$ ,  $b$ , and  $c$  are the coefficients in (5) in the terms containing  $E$  raised to the second, first, and zeroth powers, respectively. For a calculation of  $Q$ , it is convenient to define the ground-state energy in such a manner that one of the three matrix elements of the operator  $H^0$  (e.g.,  $H_{33}^0$ ) is zero. With  $V = 0$  the quantity  $Q_0$  is

$$Q_0 = \frac{-1}{108} H_{11}^0{}^2 H_{22}^0{}^2 (H_{11}^0 - H_{22}^0)^2. \quad (6)$$

For sufficiently small values of  $V$ , at least  $Q$  is obviously negative. In this case, therefore, the secular equation in (5) has three real roots, which correspond to wave functions of the type in (1), differing from each other only in the values of the coefficients  $A_1$ ,  $A_2$ , and  $A_3$ . If  $V$  is nonzero but quite small, terms proportional to  $|V_{12}|^2$  and

$|V_{13}|^2$  are added to expression (6) for  $Q$ . To determine the order of magnitude of these terms, we consider which parts are used to construct the total value of  $E$ . For this purpose, we express the coefficients  $A_2$  and  $A_3$  in the last two equations in (4) in terms of  $A_1$ , and we substitute their values into the first equation of this system. As a result, this equation becomes

$$H_{11}^0 + \frac{2|V_{12}|^2}{E - H_{22}^0} + \frac{2|V_{13}|^2}{E - H_{33}^0} = E. \quad (7)$$

If the value of  $E$  in this equation is equal to the energy of a magnetic state, then the terms on the left side of (7) have a simple physical meaning. Specifically,  $H_{11}^0$  is the sum of the eigenenergies of the degenerate electron gas and the impurity atom; the two other terms describe the energy of the interaction between these subsystems,  $E_{\text{int}}$ . The energy  $E_{\text{int}}$  is small in comparison with  $U$  if  $U \gg \Gamma$ , where  $\Gamma$  is the virtual width of the impurity atom.<sup>2</sup> It thus follows from (6) and (7) that if the differences between the energies corresponding to different magnetic states of the impurity atom are much larger than  $E_{\text{int}}$  then  $Q < 0$ .

4. A particular value of the two-particle electron-hole Green's function is given by

$$G_{-\sigma\sigma}(t_1 - t_2) = \langle 0 | T \tilde{\alpha}_\sigma(t_1) \tilde{a}_\sigma(t_2) \tilde{a}_\sigma^+(t_2) \tilde{a}_\sigma^+(t_1) | 0 \rangle, \quad (8)$$

where  $\tilde{a}_\sigma^+(t)$  and  $\tilde{a}_\sigma(t)$  are the creation and annihilation operators for an electron in a  $d$  level of the impurity atom with a spin  $\sigma$  in the Heisenberg representation, and  $T$  performs a chronological ordering of the operators. The Fourier transform of  $G_{-\sigma\sigma}(t_1 - t_2)$  is

$$G_{-\sigma\sigma}(\omega) = i \sum_n \left[ \frac{\langle 0 | a_\sigma a_\sigma^+ | n \rangle \langle n | a_{-\sigma} a_\sigma^+ | 0 \rangle}{\omega - E_n + E_0 + i \delta} - \frac{\langle 0 | a_{-\sigma} a_\sigma^+ | n \rangle \langle n | a_\sigma a_{-\sigma}^+ | 0 \rangle}{\omega + E_n - E_0 - i \delta} \right]. \quad (9)$$

The summation over  $n$  in this expression is a sum over all states of the system under consideration, with a fixed total number of particles. If we adopt a nonmagnetic state with an energy  $E_0$  as the ground state  $|0\rangle$ , then the magnetic state in the sum over  $n$  in (9) gives rise to poles at the values  $\pm(E_m - E_0)$  of  $\omega$ , where  $E_m$  is the energy of the magnetic state.

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